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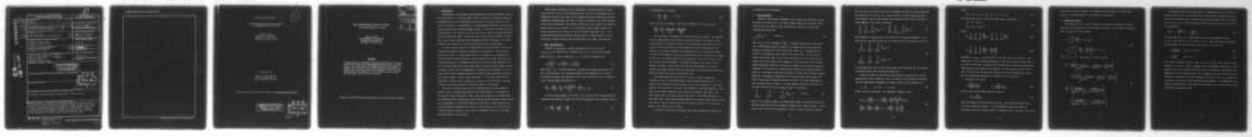

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SOME CONSIDERATIONS OF ELASTIC ANALYSES OF DISCRETE MODELS OF SOLIDS*

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ABSTRACT

The possibility is examined of studying the behavior of elastic solids on the basis of a model which considers them to be made up by a very large number of elementary particles arranged in a regular lattice array. Some of the simplifications which are needed (e.g., the neglect of surface tension) to make the analysis practical are examined, first in general terms and then for the simple case of a bar in tension.

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1. Introduction

The analysis of the stresses and deformations of solids is normally carried out on the basis of a continuum model, whether classical or exhibiting some sort of microstructure, which represents macroscopically the actual discrete structure of the material. Alternatively, a discrete model can be used, and there are then two basic ways in which one might proceed. In the first, we start from the continuum model, and replace it by a discrete one by means of suitable partitioning into appropriate units. This is the basis of very powerful methods of analysis, such as those employing finite elements or finite differences. The great value of these approaches is well known and need not be discussed here.

A second approach consists in starting with the discontinuous structure and attempting to perform calculations immediately on that basis. This has been tried (e.g.,[1,2]); in these works the body is considered to be composed of a relatively small number of material points, interactions between them being considered numerically. To represent more realistically the actual material, however, one would think that a very large number of material points should be used--so large, in fact, that a continuum may in some sense be approached. It is unlikely that a purely numerical approach is useful in this connection, because of the enormous number of points being considered; it is however possible that analytical techniques may be introduced to assist in the calulations. An examination of the latter possibility forms the subject of this paper.

The present approach starts with the consideration of a large number of material points, representing atoms and thus being assumed to be separated by distances of atomic dimensions. Atomic forces are assumed to act between them in accordance with the appropriate laws of attraction and repulsion, necessitating the establishment of equilibrium equations at each point. These equations are then simplified by neglecting the effect of surface tension [3], and by the use of Saint Venant's principle; this allows a mathematical shift to a continuum and thus solution of the problem.

This approach therefore involves postponing as long as possible the transition from the lattice to the continuum model. This has the advantage that the transition from one to the other can be examined from the standpoint of a purely mathematical approximation, and thus, at least in principle, any errors incurred can be easily ascertained. The problem chosen here is the simplest one possible, namely that of a bar in tension, and one may have serious doubts whether the present approach can be extended to any but the most elementary cases. It is nevertheless hoped that the present analysis may be of some interest in illustrating the concepts involved and the difficulties that might be encountered.

2. Basic Considerations

Consider two particles, located respectively at $P_i(x_i,y_i,z_i)$ and $P_j(x_j,y_j,z_j)$ and separated by a distance $|\vec{r}_{ij}| = r_{ij}$. Let the force between them be $\vec{F}_{ij}(r_{ij})$, and act along $\vec{r}_{ij}$, i.e., so that its components are

$$F_{ij}\left(\frac{x_j-x_i}{r_{ij}}\right) ; F_{ij}\left(\frac{y_j-y_i}{r_{ij}}\right) ; F_{ij}\left(\frac{z_j-z_i}{r_{ij}}\right) \tag{1}$$

where $|\vec{F}_{ij}| = F_{ij}$. During deformation, the particles undergo displacements $\vec{u}_i$ and $\vec{u}_j$ respectively. The consequent change in the components (1) is easily calculated, and gives the additional force between the particles, on the assumption of infinitesimal deformations, as

$$\overrightarrow{\delta F_{ij}} = \left(\frac{\partial F_{ij}}{\partial r_{ij}} - \frac{F_{ij}}{r_{ij}}\right) \frac{\vec{r}_{ij}\cdot(\vec{u}_j-\vec{u}_i)}{r_{ij}^2} - \frac{F_{ij}}{r_{ij}}\left(\vec{u}_j - \vec{u}_i\right) \tag{2}$$

It will be next assumed, as is usual [4,5], that the force between particles represents the difference between an attractive (positive) and a repulsive term, or

$$F_{jj} = \frac{\partial V}{\partial r_{ij}} = \frac{mA}{r_{ij}^{m+1}} - \frac{nB}{r_{ij}^{n+1}} \tag{3}$$

corresponding to a potential

$$V = \frac{B}{r_{ij}^{n}} - \frac{A}{r_{ij}^{m}} \quad ; \quad n > m > o \tag{3a}$$

where A and B are constants. The term in parenthesis is eq.(2) is then

$$\frac{\partial F_{ij}}{\partial r_{ij}} - \frac{F_{ij}}{r_{ij}} = \frac{n(n+2)B}{r_{ij}^{n+2}} - \frac{m(m+2)A}{r_{ij}^{m+2}} \tag{4}$$

It is now easy, in principle, to see how one should proceed: the resultant force on each particle, exerted by all other particles, is set equal to zero if the particle is internal, and equal to the appropriate applied force if the particle is on the surface (on the assumption that only surface forces are applied). Practically, however, this would give rise to a prohibitive number of equations and unknowns, and it is therefore necessary to simplify the problem. To that end, two surface effects will be neglected. The first of these is the one conventionally disregarded in continuum solutions on the basis of Saint Venant's principle, which allows the details of distribution of the forces applied over a small surface are to be overlooked, since they practically do not affect the solution outside a thin surface layer.

The second neglected effect does not arise in classical elasticity, although it arises in continuum theories exhibiting microstructure [3]. It refers to the presence of surface tension, and is also confined to a thin layer adjacent to the surface of the body. The thickness of this layer however, of the order of the atomic dimensions, and therefore much smaller than that of the Saint Venant layer, the latter being of the order of the linear dimensions of the loaded area. Hence surface tension affects an extremely small portion of the body and can safely be neglected if (as is presently desired) a solution analogous to the classical one is sought.

To clarify the above general remarks, the special example of a uniform bar

in tension will be considered.

3. A Bar in Tension

Consider a uniform bar, extending in the x-direction, and pulled in that direction by an end-force P, all other surfaces being free of applied loads. Consider first the forces in the y-direction on a generic i-th particle; equilibrium requires that

$$\sum_{\text{all } j} \delta F_{ijy} = o \qquad \text{for all } i \tag{5}$$

where δF_{ijy} is the y-component of $\vec{\delta F}_{ij}$. Assume for simplicity of discussion that the particles occupy the vertices of a simple cubic lattice, and that y=constant represents one of the free faces of the bar. Consider first the portion of the summation which refers to the y-direction: as one proceeds further and further from a face into the interior of the body, more and more planes of particles appear in the summation. This gives rise to the surface effect previously referred to, and which is limited to very few such planes; to disregard it is equivalent to neglecting the presence of a physical surface, except as a place where loads may be applied. In other words the body is mathematically considered to extend beyond its actual surface, sufficiently far that the same type of equilibrium equations hold at all planes regardless of their distance from the surface. The same argument holds for all surface of the body, and eq.(5) for our problem can then be written as:

$$\sum_{x_j=-R}^{R} \quad \sum_{y_j=-R}^{R} \quad \sum_{z_j=-R}^{R} \delta F_{ijy} = o \qquad \text{for all } i \tag{6}$$

where R is a distance chosen to be sufficiently large to include the entire bar and what additional portion is needed to eliminate the surface effects; it will be seen that, for ease of calculations, it may at times be taken as infinite.

For any value of i, the y-portion of the summation can now be separated into the two regions $y_j \leq y_i$ and $y_j > y_i$; since no forces in this direction are anywhere applied, each of these regions must separately yield a zero resultant, or (with symmetry in the other directions):

$$4\sum_{x_j=o}^{R}\sum_{y_j=-R}^{y_i}\sum_{z_j=o}^{R}\delta F_{ijy} = o \quad ; \quad 4\sum_{x_j=o}^{R}\sum_{y_j=y_{i+1}}^{R}\sum_{z_j=o}^{R}\delta F_{ijy} = o \tag{7}$$

The treatment of equilibrium in the z-direction is entirely analogous; so is that for the x-direction except for the introduction of the applied force P, or

$$4\sum_{x_j=-R}^{x_i}\sum_{y_j=o}^{R}\sum_{z_j=o}^{R}\delta F_{ijx} = P \tag{8}$$

$$4\sum_{x_j=x_{i+1}}^{R}\sum_{y_j=o}^{R}\sum_{z_j=o}^{R}\delta F_{ijx} = -P$$

In this manner the local surface effects have been eliminated, but the presence of applied surface loads has been accounted for.

Assume now, either by similarity to the classical solution or as an independent semi-inverse assumption, and on the basis of Saint Venant's principle, that the displacement components of a generic point P_i can be taken to be

$$u_i = ax_i \quad ; \quad v_i = by_i \quad ; \quad w_i = bz_i \tag{9}$$

where a and b are constants. The components of $\vec{\delta F}_{ij}$ are then

$$\delta F_{ijx} = \left[a\frac{\partial F_{ij}}{\partial r_{ij}} + (b - a)\left(\frac{\partial F_{ij}}{\partial r_{ij}} - \frac{F_{ij}}{r_{ij}}\right)\left(\frac{\eta_{ij}^2 + \xi_{ij}^2}{r_{ij}^2}\right)\right]\xi_{ij}$$

$$\frac{\delta F_{ijy}}{\eta_{ij}} = \frac{\delta F_{ijz}}{\xi_{ij}} = b\frac{\partial F_{ij}}{\partial r_{ij}} + (a - b)\left(\frac{\partial F_{ij}}{\partial r_{ij}} - \frac{F_{ij}}{r_{ij}}\right)\frac{\xi_{ij}^2}{r_{ij}^2} \tag{10}$$

where

$$\xi_{ij} = x_j - x_i \; ; \; \eta_{ij} = y_j - y_i \; ; \; \zeta_{ij} = z_j - z_i \tag{11}$$

The second ones of eqs. (7) and (8) then become, respectively,

$$\begin{aligned} bS_1 + (a - b)S_2 &= o \\ aS_1 + 2(b - a)S_2 &= P \end{aligned} \tag{12}$$

where

$$S_1 = \sum_{\xi=o}^{R} \sum_{\eta=h}^{R} \sum_{\zeta=o}^{R} \frac{\partial F_{ij}}{\partial r_{ij}} \eta = \sum_{\xi=h}^{R} \sum_{\eta=o}^{R} \sum_{\zeta=o}^{R} \frac{\partial F_{ij}}{\partial r_{ij}} \xi \tag{13a}$$

$$S_2 = \sum_{\xi=o}^{R} \sum_{\eta=h}^{R} \sum_{\zeta=o}^{R} \left(\frac{\partial F_{ij}}{\partial r_{ij}} - \frac{F_{ij}}{r_{ij}} \right) \frac{\xi^2 \eta}{r_{ij}^2} \tag{13b}$$

and where $h = \left(y_{i+1} - y_i \right)$ is the side of the basic cube in the lattice. The other forms of S_2, obtained by permutation of ξ, η and ζ, have not been shown in eq. (13b) for the sake of brevity, and the subscripts ij have been dropped from these quantities for simplicity of writing. It then appears that the first of eqs. (7) and (8) are also satisfied, because use of (12) automatically insures that the equilibrium equations are satisfied for all values of i.

Solution of (12) gives

$$a = \frac{P(S_2 - S_1)}{S_1(3S_2 - S_1)} \quad ; \quad b = \frac{PS_2}{S_1(3S_2 - S_1)} \tag{14}$$

In particular, we may define Poisson's ratio as

$$\nu = - \frac{b}{a} = \frac{S_2}{S_1 - S_2} \tag{15}$$

There now remains the evaluation of S_1 and S_2: this may be performed either in a direct numerical fashion, or in an approximate analytical manner by replacing the sum over discrete points by integrals over a continuum. The latter

approach will now be followed; it exemplifies the previously discussed transition to a continuum model at a late stage of the analysis.

4. Evaluation of Sums

The trapeziodal rule, usually employed to approximate integrals by means of sums, may be conversely used to approximate and present sums by means of integrals. Then, provided R is large enough,

$$S_1 = \int_h^R \int_h^R \frac{\partial F_{ij}}{\partial r_{ij}} \, \xi \, \pi \, r_o \, d \, r_o \, d \, \xi$$

$$S_2 = \int_h^R \int_h^R \int_h^R \left(\frac{\partial F_{ij}}{\partial r_{ij}} - \frac{F_{ij}}{r_{ij}} \right) \frac{\xi^2 \eta}{r_{ij}^2} \, d\xi \, d\eta \, d\zeta \qquad (16)$$

where $r_o^2 = \eta^2 + \zeta^2$. Then, with (3) and (4), we have

$$\frac{S_1}{\pi} = A\left(\frac{m+1}{m-2}\right)\left[\frac{2}{(R^2+h^2)^{(m-2)/2}} - \frac{1}{(\sqrt{2}\,R)^{m-2}} - \frac{1}{(\sqrt{2}\,h)^{m-2}} \right]$$

$$- B\left(\frac{n+1}{n-2}\right)\left[\frac{2}{(R^2+h^2)^{(n-2)/2}} - \frac{1}{(\sqrt{2}\,R)^{n-2}} - \frac{1}{(\sqrt{2}\,h)^{n-2}} \right] \qquad (17)$$

$$\frac{2S_2}{\pi} = A\left[\frac{(mR^2+2h^2)}{(R^2+h^2)^{m/2}\,(m-2)} - \frac{(m+2)}{2(m-2)(\sqrt{2}\,h)^{m-2}} \right]$$

$$-B\left[\frac{(nR^2+2h^2)}{(R^2+h^2)^{n/2}\,(n-2)} - \frac{(n+2)}{2(n-2)(\sqrt{2}\,h)^{n-2}} \right]$$

Evaluation of these quantities requires a knowledge of m,n,A,B, and h, as well as a choice of R. We can however derive some general information, particularly about Poisson's ratio, without such detailed knowledge, but by inserting eqs.(17) into (15), and then simplifying the resulting expression on the basis of the inequalities

$$\frac{h}{R} \ll 1 \quad ; \quad \frac{Ah^{n-m}}{B} \ll 1 \quad ; \quad \frac{Ah^{n}}{BR^{m}} \ll 1 \tag{18}$$

and recalling that $m < n$. Three cases must now be distinguished, namely: $(m > 2, n > 2)$, $(m < 2, n > 2)$, and $(m < n < 2)$; then (18) permits the expressions obtained for Poisson's ratio from eq.(15) to be reduced to:

$$\nu = \frac{n + 2}{3(n + 2)} \qquad \text{for } n > 2, \text{ any } m < n \tag{19a}$$

$$\nu = \frac{m}{m + 2} \qquad \text{for } m < n < 2 \tag{19b}$$

It is easy to see that, from eq. (19a), $(1/3) < \nu < (1/2)$, while from eq. (19b) we have $o < \nu < (1/2)$. Thus, in agreement with experimental observation, ν never exceeds 1/2, but any positive value less than 1/2 is possible. Most metals, for example, fall in the former category [5]. Analyses such as the present one can be used to determine m or n from a knowledge of Poisson's ratio, or, conversely, to predict ν on the basis of a postulated atomic behavior. The adaptation of the concepts discussed here to more complicated problems will of course have to await further work along these lines.

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